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Water adsorption and polar properties of self-assembled diphenylalanine nanotubes

P. Zelenovskiy[1,2], E. Domingues[3], M. Kornev[1], V. Slabov[3], A. Nuraeva[1], S. Vasilev[1,4], V. Yuzhakov[1], S. Kopyl[3], F.M.L. Figueiredo[3], V. Shur[1], A. Kholkin[1,3]

[1]*School of Natural Sciences and Mathematics, Ural Federal University, 620000, Ekaterinburg, Russia*

[2]*Department of Chemistry & CICECO−Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal*
zelenovskiy@urfu.ru

[3]*Department of Physics & CICECO−Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal*

[4]*Chemical Department, University of Limerick, Castletroy Limerick, Ireland*

Self-assembled micro- and nanotubes of diphenylalanine dipeptide (H-Phe-Phe-OH, FF) represent promising functional biomaterial for new medical and energy harvesting devices [1] due to its outstanding piezoelectric [1, 2], pyroelectric [3] and mechanical [4] properties. After the self-assembly in aqueous solution water molecules remain captured inside the nanochannels, stabilize its structure [5] and modify physical properties. Here we studied water adsorption in FF nanochannels, its structure and polar properties.

Room temperature nitrogen and water adsorption measurements showed that the specific surface area of FF nanotubes is comparable with that of polymers of intrinsic microporosity, several kinds of metal-organic frameworks and porous carbons. Single-crystal X-ray diffraction and computer modeling revealed the reconstruction of the bound water layer at low temperatures, whereas the peptide shell remains almost the same. Temperature of this reconstruction corresponds to a phase transition observed recently at 230 K by dielectric measurements [6]. Ab-initio calculations showed that all analyzed water structures are polar, and the direction and values of their dipole moments were obtained. For all temperatures the dipole moment is mainly oriented along the nanotube's axis and is opposite to the dipole moment of the peptide shell, thus reducing the total polarization of the nanotube. However, the direct piezoelectric measurements demonstrated non-monotonous decrease of the piezoelectric coefficient with water removing. The origin of this contradiction is not clear yet.

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1. A. Kholkin, N. Amdursky et al., *ACS Nano* **4**, 610 (2010).
2. S. Vasilev, et al., *J. Phys. Chem. Solids* **93**, 68 (2016).
3. A. Esin, et al., *Appl. Phys. Lett.* **109**, 142902 (2016).
4. I. Azuri, L. Adler-Abramovich et al., *J. Am. Chem. Soc.* **136**, 963 (2014).
5. T. Andrade-Filho, T. Martins et al., *Theor. Chem. Acc.* **135**, 185 (2016).
6. F. Salehli, D. Chovan et al., Submitted *Adv. Funct. Mater*. (2019).